Field-scale modeling of nanoparticle transport in aquifer systems

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Authors: *Tosco, Tiziana (Politecnico di Torino - DIATI, Torino, Italy); Bianco, Carlo; Sethi, Rajandrea (Politecnico di Torino - DIATI, Torino, Italy)*

Despite their great potential for technological applications, engineered nanoparticles (NPs) can represent a significant, and still largely unknown, environmental hazard. NPs-containing products are already widely available on the market, or expected in few years, likely leading to the dissemination of large amounts of NPs in the environment. Moreover, injection into the subsurface of suspensions of iron-based micro and nanoparticles have proved promising for groundwater remediation (1). In both cases, a full understanding of the mechanisms governing the transport of NPs in the subsurface and quantitative modeling tools are necessary, for both the design of NP-based remediation technologies, and long-term fate prediction.

NP transport in porous media is controlled by particle-particle and particle-collector interactions, typically modelled with kinetic terms of deposition onto the porous medium and corresponding release. Ionic strength and flow rate play a major role in both (2). In this work, two modeling tools, MNMs and MNM3D, are proposed to simulate NP transport in porous media, respectively at laboratory and field scale, under space- and time-variable ionic strength and flow velocity. Applications of the tools are also presented. MNMs is a Matlab-based software (www.polito.it/groundwater/software/MNMs.php) implementing numerical solutions for lab-scale (1D columns) and pilot-scale NP transport (injection through a single well, radial geometry) (3-4). MNM3D is a modified version of the well-known transport model RT3D, and solves particle transport in 3-dimensional geometries (5-6). MNM3D can be used for multi-dimensional simulations and employed in many practical field-scale applications, eg. the preliminary design of in situ aquifer remediation via NP injection, and the estimate of long-term fate of NPs released in landfill leachate.

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